열간 Roll to Flat Imprint 공정에 관한 수치적 모델링 연구
Analytical Modeling of Roll to Flat Thermal Imprinting Processes for Large-Area Micro-Pattern Replication

*#송정한 [1], 란수화이 [1], 이혜진 [1], 박진호 [1], 이낙규 [1], 이근안 [1]
*#J. H. Song(jhsong@kitech.re.kr)[1], Shuhuai Lan[1] , H. J. Lee[1] , J. H. Park [1] , N. K. Lee [1], G. A. Lee [1]
[1] 한국생산기술연구원 융합생산기술연구부

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1. Introduction

Continuous roller-pressing process such as roll-to-roll (R2R, roller mold + roller pressing) or roll-to-flat (R2F, flat mold + roller pressing), has been currently applied in some industrial fields, such as gravure printing or flexography printing (or flexo). It is used to imprint intended patten on flexible thin films continuously. The replicated pattern is transferred from the roller mold or flat mold onto the surface of substrate. In the field of micro-/nano-fabrication, S. Y. Chou group firstly proposed the combination of imprinting and roller-pressing and then developed roller nanoimprint lithography (RNIL) process for rapid pattern replication on a large area substrate. Such RNIL process provides advantages such as simple equipment, lower imprint force, better replication uniformity because only a line area is in contact during imprinting. However, the continuous roller-pressing imprinting process for the fabrication of micro-pattern on the polymer substrate has not been investigated adequately and most of them are based on ultraviolet-curing techniques. For the thermal continuous imprinting process, most of investigations focus on the system development and experimental study. Few studies have been reported the filling mechanism in roller-pressing type imprinting process. In order to have a better understanding of polymer material flow behavior in the roller-pressing type imprinting process, it is necessary to establish a criterion of evaluation for roller-pressing type imprinting process.

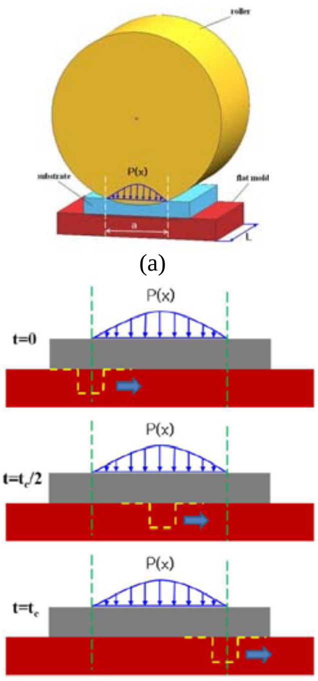
In this study we aim to develop an analytical model for the cavity-filling of polymer flow in roll-to-flat (R2F) imprinting process, which is derived based on Hertz contact pressure distribution and Navier-Stokes equation. Our goal is to obtain a relationship between process control parameters and process result. Based on a lab-scaled prototype of a R2F micro thermal imprint system, the feasibility of the model is evaluated for the micro-pattern replication over large area on polymer substrate. Series of tests were conducted to investigate the effects of process control parameters, i.e. rolling speed and loading pressure on the replication ratio on polycarbonate (PC) substrate.

2. Analytical Model

In the conventional flat-pressing type imprinting process, the loading pressure between mold and substrate is usually regarded as constantly static and uniform. However, as shown in the Fig.1 (a), in the R2F imprinting process, under the pressing of roller, the pressure distribution is the function of distance to the central contact point. In one dimension and for slow rolling, according to Hertz contact solution, the pressure distribution is given by:

$$P(x)=\frac{8F}{\pi a^2 L}\left[\left(\frac{a}{2}\right)^2-x^2\right]^{1/2} \qquad (1)$$

where *P(x)* is the pressure distribution, *F* is the normal applied force, *a* is the contact length and *L* is width of the roller as well as the flat mold.



(a)

(b)

Fig. 1 Schematic diagram of the contact model in the R2F imprint process: (a) geometrical configuration (b) pressure distribution as function of time

For every small mold cavity in the contact area, the rolling motion of roller is equivalent with the motion which the roller is fixed (only rotating with its center axis) while the flat mold moves forward, as shown in Fig.1 (b).

For every small mold cavity in the contact area, the rolling motion of roller is equivalent with the motion which the roller is fixed (only rotating with its center axis) while the flat mold moves forward, as shown in Fig.1 (b). Noting t_c as one contact time cycle, then t_c is expressed as: $t_c = a/v$, where v is the moving speed of flat mold, which is also the web speed of the roller. As presented in Eq. (1), therefore, the pressure distribution applied on every mold cavity can be expressed as function of time as the roller rolling forward in the contact area:

$$P(t)=\frac{8F}{\pi a^2 L}\left[\left(\frac{a}{2}\right)^2-\left(-\frac{a}{2}+vt\right)^2\right]^{1/2} \quad (0 \le t \le t_c) \qquad (2)$$

The material flow behavior is governed by Navier-Stokes equation:

$$\nabla P=\eta\nabla^2 V \qquad (3)$$

Neglecting the gravity effect since the material is very thin, the flow behavior equation can be expressed as:

$$\frac{\partial P}{\partial z}=-\eta\frac{\partial^2 u_z}{\partial x^2} \qquad (4)$$

where $\partial P/\partial z$ is the pressure gradient, η is the viscosity, and u_z is the flow velocity in *z*-direction. Solving for u_z with a “no-slip” boundary condition at the cavity walls, In order to simplify the analytical model, we use an average flow velocity along the cavity width in one contact time cycle. Combining equation (2) we have:

$$\bar{u}_z = \frac{1}{t_c}\frac{1}{w}\int_0^{t_c}\int_{-w/2}^{w/2} u_z dxdt = -\frac{\bar{P}}{\Delta z}\frac{w^2}{12\eta} \qquad (5)$$

where $\bar{P} = F / La$ is the average pressure over the whole contact area in one contact time cycle.

In one contact time cycle, the filling pattern height can be calculated as:

$$\Delta z = w\left(-\frac{\bar{P}a}{12v\eta}\right)^{1/2} \qquad (6)$$

Defining replication ratio as $R_{replication} = \Delta z / H$ and aspect ratio as $r_{aspect} = H / w$ and combining with equation (6) we have:

$$R_{replication} = \frac{1}{r_{aspect}}\left(-\frac{\bar{P}a}{12v\eta}\right)^{1/2} \qquad (7)$$

From equation (7), the replicating result in R2F thermal imprinting process, i.e. replication ratio $R_{replication}$, is the function of cavity aspect ratio, loading pressure, rolling speed as well as polymer viscosity, which is the function of temperature. For a certain roll-to-flat imprint system and a given flat mold, the roller diameter and contact length as well as the cavity aspect ratio are constant. Under the specific process conditions, i.e. loading pressure, rolling speed and imprinting temperature, we can approximately calculate the replication ratio.

3. Experimental Comparison

The analytical model is evaluated by comparing the model prediction with the experiment result of replication ratio, in which one process parameter varies while others are kept constant. According to equation (7), replication ratio would decrease as rolling speed increases because material flow filling time gets shorter. And the predicted replication ratio would increase with the increasing of loading pressure and temperature since the increase of loading pressure can ensure more material filled into the pattern cavity.

In order to study the effect of rolling speed, the speed was varied from 0.2 mm/s to 2 mm/s whereas temperature and loading pressure were kept constant, which are 160 ºC and 7.5 MPa, respectively. After experiments, the imprinted PC substrates were measured at several points over the whole surface area to calculate the average measured replication ratio. Fig.2 shows the comparison between experimental data and analytical model prediction. In the figure it can be found there is consistent tendency between the experimental data and model prediction.

For the evaluation of the effect of loading pressure, the pressure was varied from 5.5 MPa to 11.5 MPa whereas temperature and rolling speed were kept constant at 160 ºC and 0.2 mm/s respectively. The analytical model can predict the process result with these parameters. The comparison between experimental data and analytical model prediction is shown in Fig.8. From the figure it is found that consistent tendency between the experimental data and model prediction. As the loading pressure increases from 5.5 MPa to 11.5 MPa, the replication ratio gradually increases from approximately 50% to 70%. It is because higher loading pressure can drive the material flow faster and a higher filling velocity. Thus, greater replication ratio can be achieved.

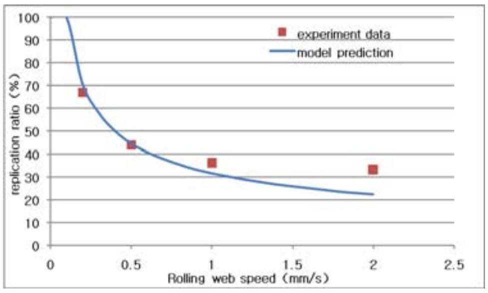


Fig.2 Comparison of model prediction and experiment data: relationship between rolling speed and replication ratio

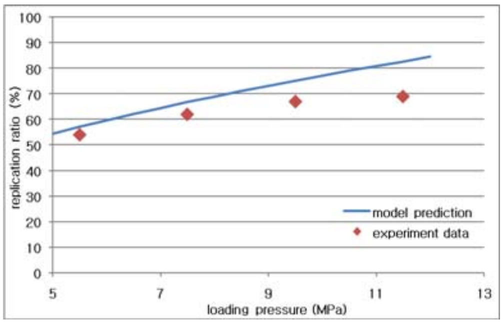


Fig.3 Comparison of model prediction and experiment data: relationship between loading pressure and replication ratio

4. Conclusion

In summary, we have demonstrated a R2F thermal imprinting process to address the increasing demand for large-area micro-pattern replication on polymer substrate. In this paper, we developed an analytical model for the cavity-filling of polymer flow in roll-to-flat (R2F) imprinting process for predicting the replication ratio as a as a function of process control parameters, i.e. imprinting pressure and rolling speed. Subsequently, series of experiments were carried out using a flat mold and commercially available polycarbonate substrates to evaluate the feasibility of analytical model and R2F micro thermal imprint system as well as process control parameters' effect. The developed analytical model of polymer flow behavior has reasonable agreement with the experimental data, indicating that the analytical model could be used for predicting the process results.

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